FIGURE 1

Amino acid sequence for full-length human wild type DPPIV [SEQ- ID No.NO: 1] (Residues 39-766 are underlined)

MKTPWKVLLG	LLGAAALVTI	ITVPVVLLNK	GTDDATAD <u>SR</u>	KTYTLTDYLK	NTYRLKLÝSL	60
RWISDHEYLY	KQENNILVFN	AEYGNSSVFL	ENSTFDEFGH	SINDYSISPD	GQFILLEYNY	120
VKQWRHSYTA	SYDIYDLNKR	QLITEERIPN	NTQWVTWSPV	GHKLAYVWNN	DIYVKIEPNL	180
PSYRITWTGK	EDIIYNGITD	WVYEEEVFSA	YSALWWSPNG	TFLAYAQFND	TEVPLIEYSF	240
YSDESLQYPK '	TVRVPYPKAG	AVNPTVKFFV	VNTDSLSSVT	NATSIQITAP	ASMLIGDHYL	300
CDVTWATQER	ISLQWLRRIQ	NYSVMDICDY	DESSGRWNCL	VARQHIEMST	TGWVGRFRPS	360
EPHFTLDGNS	FYKIISNEEG	YRHICYFQID	KKDCTFITKG	TWEVIGIEAL	TSDYLYYISN	420
EYKGMPGGRN I	LYKIQLSDYT	KVTCLSCELN	PERCQYYSVS	FSKEAKYYQL	RCSGPGLPLY	480
TLHSSVNDKG	LRVLEDNSAL	DKMLQNVQMP	SKKLDFIILN	ETKFWYQMIL	PPHFDKSKKY	540
PLLLDVYAGP (CSQKADTVFR	LNWATYLAST	ENIIVASFDG	RGSGYQGDKI	MHAINRRLGT	600
FEVEDQIEAA I	RQFSKMGFVD	NKRIAIWGWS	YGGYVTSMVL	GSGSGVFKCG	IAVAPVSRWE	660
YYDSVYTERY I	MGLPTPEDNL	DHYRNSTVMS	RAENFKQVEY	LLIHGTADDN	VHFQQSAQIS	720
KALVDVGVDF (QAMWYTDEDH	GIASSTAHQH	IYTHMSHFIK	QCFSLP		766

Amino acid sequence for residues 39-766 of DPPIV with a N-terminal 6x-histidine tag [SEQ: ID No: NO: 3] (part of a gp67 signal sequence and a 6x-histidine tag is underlined)

ADPGGSHHHH HHSRKTYTLT DYLKNTYRLK LYSLRWISDH EYLYKQENNI LVFNAEYGNS 60 SVFLENSTFD EFGHSINDYS ISPDGQFILL EYNYVKQWRH SYTASYDIYD LNKRQLITEE 120 RIPNNTQWVT WSPVGHKLAY VWNNDIYVKI EPNLPSYRIT WTGKEDIIYN GITDWVYEEE 180 VFSAYSALWW SPNGTFLAYA OFNDTEVPLI EYSFYSDESL QYPKTVRVPY PKAGAVNPTV 240 KFFVVNTDSL SSVTNATSIQ ITAPASMLIG DHYLCDVTWA TQERISLQWL RRIQNYSVMD 300 ICDYDESSGR WNCLVAROHI EMSTTGWVGR FRPSEPHFTL DGNSFYKIIS NEEGYRHICY 360 FQIDKKDCTF ITKGTWEVIG IEALTSDYLY YISNEYKGMP GGRNLYKIQL SDYTKVTCLS 420 CELNPERCQY YSVSFSKEAK YYQLRCSGPG LPLYTLHSSV NDKGLRVLED NSALDKMLQN 480 VQMPSKKLDF IILNETKFWY QMILPPHFDK SKKYPLLLDV YAGPCSQKAD TVFRLNWATY 540 LASTENIIVA SFDGRGSGYQ GDKIMHAINR RLGTFEVEDQ IEAARQFSKM GFVDNKRIAI 600 WGWSYGGYVT SMVLGSGSGV FKCGIAVAPV SRWEYYDSVY TERYMGLPTP EDNLDHYRNS 660 TVMSRAENFK QVEYLLIHGT ADDNVHFQQS AQISKALVDV GVDFQAMWYT DEDHGIASST 720 AHOHIYTHMS HFIKOCFSLP 740

FIGURE 1 (Cont.)A

Human cDNA sequence encoding residues 39-766 of DPPIV [SEQ: ID No. 2NO: 3]

AGTCGCAAAA	CTTACACTCT	AACTGATTAC	TTAAAAAATA	CTTATAGACT	GAAGTTATAC	60
TCCTTAAGAT	GGATTTCAGA	. TCATGAATAT	CTCTACAAAC	AAGAAAATAA	TATCTTGGTA	120
TTCAATGCTG	AATATGGAAA	CAGCTCAGTT	TTCTTGGAGA	ACAGTACATT	TGATGAGTTT	180
GGACATTCTA	TCAATGATTA	TTCAATATCT	CCTGATGGGC	AGTTTATTCT	CTTAGAATAC	240
AACTACGTGA	AGCAATGGAG	GCATTCCTAC	ACAGCTTCAT	ATGACATTTA	TGATTTAAAT	300
AAAAGGCAGC	TGATTACAGA	AGAGAGGATT	CCAAACAACA	CACAGTGGGT	CACATGGTCA	360
CCAGTGGGTC	ATAAATTGGC	ATATGTTTGG	AACAATGACA	TTTATGTTAA	AATTGAACCA	420
AATTTACCAA	GTTACAGAAT	CACATGGACG	GGGAAAGAAG	ATATAATATA	TAATGGAATA	480
ACTGACTGGG	TTTATGAAGA	GGAAGTCTTC	AGTGCCTACT	CTGCTCTGTG	GTGGTCTCCA	540
AACGGCACTT	TTTTAGCATA	TGCCCAATTT	AACGACACAG	AAGTCCCACT	TATTGAATAC	600
TCCTTCTACT	CTGATGAGTC	ACTGCAGTAC	CCAAAGACTG	TACGGGTTCC	ATATCCAAAG	660
GCAGGAGCTG				ATACAGACTC	TCTCAGCTCA	720
GTCACCAATG	CAACTTCCAT	ACAAATCACT	GCTCCTGCTT	CTATGTTGAT	AGGGGATCAC	780
TACTTGTGTG	ATGTGACATG	GGCAACACAA	GAAAGAATTT	CTTTGCAGTG	GCTCAGGAGG	840
ATTCAGAACT	ATTCGGTCAT	GGATATTTGT	GACTATGATG	AATCCAGTGG	AAGATGGAAC	900
TGCTTAGTGG	CACGGCAACA	CATTGAAATG	AGTACTACTG	GCTGGGTTGG	AAGATTTAGG	960
CCTTCAGAAC	CTCATTTTAC	CCTTGATGGT	AATAGCTTCT	ACAAGATCAT	CAGCAATGAA	1020
GAAGGTTACA	GACACATTTG	CTATTTCCAA	ATAGATAAAA	AAGACTGCAC	ATTTATTACA	1080
AAAGGCACCT	GGGAAGTCAT	CGGGATAGAA	GCTCTAACCA	GTGATTATCT	ATACTACATT	1140
AGTAATGAAT	ATAAAGGAAT	GCCAGGAGGA	AGGAATCTTT	ATAAAATCCA	ACTTATTGAC	1200
TATACAAAAG	TGACATGCCT	CAGTTGTGAG	CTGAATCCGG	AAAGGTGTCA	GTACTATTCT	1260
GTGTCATTCA	GTAAAGAGGC	GAAGTATTAT	CAGCTGAGAT	GTTCCGGTCC	TGGTCTGCCC	1320
CTCTATACTC	TACACAGCAG	CGTGAATGAT	AAAGGGCTGA	GAGTCCTGGA	AGACAATTCA	1380
GCTTTGGATA	AAATGCTGCA	GAATGTCCAG	ATGCCCTCCA	AAAAACTGGA	CTTCATTATT	1440
TTGAATGAAA	CAAAATTTTG	GTATCAGATG	ATCTTGCCTC	CTCATTTTGA	TAAATCCAAG	1500
AAATATCCTC	TACTATTAGA			GTCAAAAAGC		1560
TTCAGACTGA	ACTGGGCCAC	TTACCTTGCA	AGCACAGAAA	ACATTATAGT	AGCTAGCTTT	1620
				ATGCAATCAA		1680
GGAACATTTG	AAGTTGAAGA	TCAAATTGAA	GCAGCCAGAC	AATTTTCAAA	AATGGGATTT	1740
GTGGACAACA	AACGAATTGC	AATTTGGGGC	TGGTCATATG	GAGGGTACGT	AACCTCAATG	1800
GTCCTGGGAT	CGGGAAGTGG	CGTGTTCAAG	TGTGGAATAG	CCGTGGCGCC	TGTATCCCGG	1860
TGGGAGTACT	ATGACTCAGT	GTACACAGAA	CGTTACATGG	GTCTCCCAAC	TCCAGAAGAC	1920
AACCTTGACC	ATTACAGAAA	TTCAACAGTC	ATGAGCAGAG	CTGAAAATTT	TAAACAAGTT	1980
GAGTACCTCC	TTATTCATGG	AACAGCAGAT	GATAACGTTC	ACTTTCAGCA	GTCAGCTCAG	2040
ATCTCCAAAG	CCCTGGTCGA	TGTTGGAGTG	GATTTCCAGG	CAATGTGGTA	TACTGATGAA	2100
			CAACATATAT	ATACCCACAT	GAGCCACTTC	2160
ATAAAACAAT	GTTTCTCTTT	ACCT				2184

FIGURE 3

LEGEND

Column headings from left to right are (A) 'Atom Number', (B) 'Atom Type', (C) 'Amino Acid', (D) 'Chain Identifier', (E) 'Amino Acid Number' (reference to SEQ ID NO: 3), (F) 'X Coordinate', (G) 'Y Coordinate', (H) 'Z Coordinate', (I) 'Occupancy' (OCC) and (J) 'B factor'.

Α	В	C	D E	F	G	H	I	J
1	N	ARG A		-78.499	25.732	64.898		51.08
2	CA	ARG A		-77.682	24.936	63.934		50.91
3	CB	ARG A		-76.853	25.895	63.064		51.59
4	CG	ARG A	52 14	-76.507	25.382	61.666		54.33
5	CD	ARG A	52 14	-76.170	26.503	60.678	1.00	
6	NE	ARG A	5214	-76.489	26.159	59.292		61.47
7	cz	arg a	52 14	-76.158	26.909	58.245		62.24
8	NH1	ARG A	52 14	-75.492	28.043	58.429	1.00	61.77
9	NH2	ARG A	52 14	-76.486	26.525	57.016	1.00	62.51
10	C	ARG A	52 14	-76.763	23.943	64.655	1.00	49.68
11	0	ARG A	$\frac{52}{14}$	-75.871	23.360	64.038		49.98
12	N	LYS A	53 15	-76.986	23.740	65.952	1.00	
13	CA	LYS A	53 15	-76.091	22.892	66.731	1.00	46.49
14	CB	LYS A	53 <u>15</u>	-75.983	23.350	68.181	1.00	46.98
15	CG	LYS A	53 15	-77.288	23.731	68.859	1.00	
16	CD	LYS A	53 15	-77.002	24.390	70.224	1.00	53.43
17	CE	LYS A	53 15	-78.085	25.406	70.605	1.00	55.57
18	NZ	LYS A	53 15	-77.642	26.378	71.671	1.00	57.35
19	C	LYS A	53 <u>15</u>	-76.358	21.398	66.670	1.00	44.72
20	0	LYS A	53 15	-77.487	20.943	66.476	1.00	44.71
21	N	THR A	54 16	-75.279	20.641	66.812	1.00	42.33
22	CA	THR A	$\frac{54}{16}$	-75.363	19.201	66.815	1.00	39.34
23	CB	THR A	54 16	-74.225	18.582	66.009	1.00	39.46
24	OG1	THR A	54 16	-72.972	18.975	66.565	1.00	38.25
25	CG2	THR A	<u>5416</u>	-74.187	19.163	64.603	1.00	38.11
26	C	THR A	54 16	-75.295	18.761	68.251	1.00	37.67
27	0	THR A	. 54 16	-75.098	19.578	69.150	1.00	37.00
28	N	TYR A	55 17	-75.534	17.476	68.466	1.00	35.46
29	CA	TYR A	55 17	-75.439	16.896	69.785	1.00	33.88
30	CB	TYR A	<u>5517</u>	-76.340	15.666	69.865	1.00	33.82
31	CG	TYR A	55 17	-76.311	14.944	71.179	1.00	32.28
32	CD1	TYR A	55 17	-77.203	15.265	72.191	1.00	32.55
33	CEl	TYR A	55 17	-77.170	14.603	73.411	1.00	32.32
34	CZ	TYR A	55 <u>17</u>	-76.248	13.588	73.600	1.00	31.27
35	OH	TYR A	55 17	-76.199	12.905	74.782	1.00	29.92
36	CE2	TYR A	5517	-75.366	13.257	72.606	1.00	30.87
37	CD2	TYR A	55 <u>17</u>	-75.395	13.936	71.405		30.90
38	C	TYR A	55 17	-73.971	16.526	69.924	1.00	32.90
39	0	TYR A	55 17	-73.501	15.626	69.247	1.00	32.98
40	M	THR A	56 18	-73.247	17.244	70.776		31.58
41	CA	THR A	56 18	-71.792	17.060	70.901	1.00	30.40

FIGURE 3 (Cont.)A

A	В	С	D	E	F	G	н	I	J
42	CB	THE	A.	5618	-71.126	18.369	71.311	1.00	29.92
43	OG1	THE	A	56 18	-71.551	18.690	72.644	1.00	29.95
44	CG2	THE	A	56 18	-71.606	19.526	70.444	1.00	30.35
45	C	THE	Α	56 18	~71.353	16.053	71.937	1.00	29.51
46	0	THE	A	56 18	-72.131	15.625	72.782	1.00	28.96
47	N	LEU	A	57 19	-70.064	15.739	71.895	1.00	29.18
48	CA	LEU	I A	57 19	-69.454	14.841	72.858	1.00	29.40
49	CB	LEU	A	5719	-67.958	14.681	72.570	1.00	29.30
50	CG	LEU	Α	57 19	-67.186	13.725	73.475	1.00	29.28
51	CD1	LEU	Ą	5719	-67.668	12.278	73.289	1.00	26.89
52	CD2	LEU	Α	57 19	-65.706	13.844	73.171	1.00	29.54
53	C	LEU	Α	57 19	-69.668	15.422	74.247	1.00	29.40
54	0	LEU	A	57 19	-70.014	14.702	75.174	1.00	29.52
55	Ŋ	THR	. A	58 20	-69.483	16.731	74.375	1.00	29.38
56	CA	THR	A	58 20	-69.674	17.419	75.650	1.00	29.71
57	CB	THR	Α	5820	-69.270	18.921	75.530	1.00	30.55
58	OG1	THR	A	58 20	-67.858	19.022	75.275	1.00	31.86
59	CG2	THR	Α	58 20	-69.426	19.646	76.871	1.00	29.63
60	C	THR	A	58 20	-71.095	17.286	76.152	1.00	29.39
61	0	THR	Α	58 20	-71.311	17.062	77.336	1.00	29.75
62	N	ASP	A	59 21	-72.070	17.413	75.255	1.00	29.23
63	CA	ASP	Α	59 21	-73.467	17.237	75.640	1.00	28.50
64	CB	ASP	A	59 21	-74.381	17.347	74.420	1.00	28.92
65	CG	ASP	Α	59 21	-74.390	18.740	73.824	1.00	30.30
66	OD1	ASP	A	5921	-74.348	19.699	74.612	1.00	30.33
67	OD2	ASP	A	59 21	-74.419	18.969	72.588	1.00	31.62
68	C	ASP	Α	59 21	-73.635	15.871	76.288	1.00	28.19
69	0	ASP	A	5921	-74.255	15.737	77.363	1.00	27.07
70	N	TYR	A	60 22	-73.067	14.854	75.635	1.00	28.18
71	CA	TYR	Α	60 22	-73.110	13.498	76.162	1.00	28.06
72	CB	TYR	A	6022	~72.478	12.503	75.180	1.00	28.13
73	CG	TYR	A	6022	-72.316	11.105	75.757	1.00	28.21
74	CD1	TYR	A	60 22	-73.381	10.473	76.387	1.00	27.52
75	CE1	TYR	Α	6022	-73.231	9.225	76.941	1.00	31.17
76	CZ	TYR	A	6022	-71.994	8.574	76.850	1.00	31.00
77	OH	TYR	A	6022	-71.855	7.320	77.396	1.00	33.09
78	CE2	TYR	A	6022	-70.920	9.184	76.231	1.00	27.37
79	CD2	TYR	A	6022	-71.086	10.444	75.703	1.00	27.39
80	C	TYR	Α	60 22	-72.400	13.430	77.507	1.00	28.37
81	0	TYR	A	60 22	-72.966	12.974	78.504	1.00	28.20
82	N	LEU	A	61 23	-71.160	13.894	77.544	1.00	29.10
83	CA	LEU	A	61 23	-70.363	13.783	78.766	1.00	29.84
84	CB	LEU	A	61 23	-68.895	14.060	78.490	1.00	29.67
85	CG	LEU	Д	61 23	~68.233	13.147	77.454	1.00	30.09
86	CD1	LEU	A	61 23	-66.745	13.421	77.442	1.00	
87	CD2	LEU	A	6123	-68.502	11.647	77.730	1.00	29.29
88	C	LEU	A	61 23	-70.846	14.639	79.919	1.00	
89	0	LEU		61 23	-70.704	14.254	81.081	1.00	
90	N	LYS	Α	52 24	-71.417	15.798	79.613	1.00	
91	CA	LYS		6224	-71.909	16.658	80.669	1.00	
92	CB	LYS	A	62 24	-71.501	18.129	80.433	1.00	33.11

FIGURE 3-(Cont.)B

93 CG LYS A 6224	A	В	C D	E	F	G	Н	I	J
95 CB LYS 66224 -69.297 17.906 81.648 1.00 32.14 96 NZ LYS A 6224 -67.820 18.355 81.702 1.00 32.14 97 C LYS A 6224 -73.426 16.521 80.864 1.00 34.49 98 O LYS A 6224 -73.426 16.521 80.864 1.00 34.49 99 N ASN A 6325 -75.517 15.506 80.214 1.00 34.15 100 CA ASN A 6325 -75.517 15.506 80.214 1.00 37.50 101 CB ASN A 6325 -75.131 14.898 81.583 1.00 38.04 101 CG ASN A 6325 -75.137 13.437 81.686 1.00 37.50 102 ASN A 6325 -75.285 12.919 <	93	CG	LYS A	. 62 24	-69.997	18.373	80.362	1.00	31.71
95 CE LYS A 6224 (67.82) 1.06 1.07 21.00 32.14 96 NZ LYS A 6224 (62.42) -67.002 17.666 82.769 1.00 29.53 98 C LYS A 6224 (73.98) 17.135 81.752 1.00 34.49 99 N ASN A 6325 (73.18) -74.082 15.701 80.048 1.00 36.15 101 CB ASN A 6325 (75.517) 15.506 80.214 (10.0) 37.50 101 CB ASN A 6325 (75.517) 15.506 80.214 (10.0) 37.50 103 ODI ASN A 6325 (75.195) 12.919 (27.93) 81.00 42.50 104 ND2 ASN A 6325 (75.195) 12.919 (27.93) 80.534 (10.0) 46.50 105 C ASN A 6325 (75.195) 12.919 (27.73) 80.534 (10.0) 40.0 46.50 106 O ASN A 6325 (75.195) 775.285 (12.75) 80.534 (10.0) 40.0 46.50 107 N THR A				-	-69.297	17.906	81.648	1.00	32.14
97 C LYS 6+224 -73.426 16.521 80.864 1.00 34.49 98 O LYS 6+224 -73.998 17.135 81.752 1.00 34.44 99 N ASN 6+225 -75.517 15.506 80.214 1.00 37.50 101 CB ASN 6+325 -75.17 15.506 80.214 1.00 38.04 102 CG ASN 6+325 -75.197 13.437 81.563 1.00 48.50 104 NDI ASN 6+325 -75.195 12.919 82.793 1.00 46.50 104 NDI ASN 6+325 -75.195 12.919 82.793 1.00 46.50 105 C ASN 6+325 -75.195 12.919 82.793 1.00 46.50 106 ASN 6+325 -75.195 12.919 82.793 1.00 30.418 107 THR 6426 <td></td> <td></td> <td></td> <td>min/man/manin</td> <td></td> <td></td> <td>81.702</td> <td></td> <td></td>				min/man/manin			81.702		
98 O LYS A 6224	96	NZ	LYS A	6224	-67.002	17.666	82.769	1.00	29.53
99 N ASN A 6325 -74.082 15.701 80.048 1.00 34.44 99 N ASN A 6325 -75.517 15.506 80.214 1.00 37.50 101 CB ASN A 6325 -75.517 15.506 80.214 1.00 37.50 101 CB ASN A 6325 -75.813 14.898 81.583 1.00 38.04 102 CG ASN A 6325 -75.97 13.437 81.686 1.00 42.36 103 OD1 ASN A 6325 -75.195 12.919 82.793 1.00 46.50 104 ND2 ASN A 6325 -75.195 12.919 82.793 1.00 46.50 104 ND2 ASN A 6325 -75.195 12.919 82.793 1.00 46.50 106 O ASN A 6325 -76.312 16.808 80.032 1.00 37.71 106 O ASN A 6325 -76.312 16.808 80.032 1.00 37.63 107 N THR A 6426 -76.066 17.493 78.926 1.00 38.29 108 CA THR A 6426 -76.066 17.493 78.926 1.00 38.29 108 CA THR A 6426 -76.666 17.493 78.926 1.00 38.89 110 CG1 THR A 6426 -76.659 19.227 77.281 1.00 39.01 110 CG1 THR A 6426 -76.817 20.607 76.955 1.00 39.02 112 C THR A 6426 -76.817 20.607 76.955 1.00 39.02 112 C THR A 6426 -76.817 20.607 76.955 1.00 39.02 113 O THR A 6426 -79.066 19.157 79.198 1.00 39.02 114 N TYR A 6527 -80.169 16.771 76.044 1.00 39.58 115 CA TYR A 6527 -80.169 16.771 76.044 1.00 39.58 115 CA TYR A 6527 -80.169 16.771 76.044 1.00 39.58 115 CA TYR A 6527 -80.169 16.771 76.044 1.00 39.51 115 CA TYR A 6527 -80.169 16.771 76.044 1.00 39.52 117 CG TYR A 6527 -80.169 16.771 76.044 1.00 39.35 115 CA TYR A 6527 -80.169 16.771 76.044 1.00 39.52 117 CG TYR A 6527 -80.106 20.166 74.431 1.00 39.35 115 CA TYR A 6527 -80.006 20.166 74.431 1.00 38.77 118 CD1 TYR A 6527 -80.006 20.166 74.431 1.00 38.78 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.78 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 38.93	97	C	LYS A	6 2 24	-73.426	16.521	80.864	1.00	34.49
100	98	0	LYS A		-73.998	17.135	81.752	1.00	34.44
101	99	N	ASN A	6325	-74.082	15.701	80.048	1.00	36.12
102	100	CA	ASN A	63 25	-75,517	15.506	80.214	1.00	37.50
103 OD1	101	CB	ASN A	53 25	-75.813	14.898	81.583	1.00	38.04
104 ND2	102	CG	ASN A	63 25	-75.397	13.437	81.686	1.00	42.36
105	103		ASN A		-75.195	12.919	82.793	1.00	46.50
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	104	ND2	ASN A	6325	-75.285	12.753	80.534	1.00	46.18
107	105	C	asn a	6325	-76.312	16.808	80.032	1.00	37.71
108 CA THR A 6426 -76.761 18.725 78.622 1.00 38.88 109 CB THR A 6426 -76.259 19.227 77.281 1.00 39.01 110 OG1 THR A 6426 -76.859 19.227 77.281 1.00 39.02 111 CG2 THR A 6426 -76.857 10.607 76.955 1.00 39.02 112 C THR A 6426 -79.066 19.157 79.198 1.00 39.02 114 N TYR A 6527 -80.017 17.410 77.514 1.00 39.93 115 CA TYR A 6527 -80.017 17.110 77.518 1.00 39.99 116 CB TYR A 6527 -80.0169 16.771 76.044 1.00 39.95 117 CG TYR A 6527 -80.438 19.087 75.151 1.00 39.25 119	106	0	ASN A	6325	-77.122	17.187	80.870	1.00	37.63
109 CB THR A 6426 -76.259 19.227 77.281 1.00 39.01 110 OG1 THR A 6426 -74.854 19.444 77.377 1.00 39.08 111 CG2 THR A 6426 -76.817 20.607 76.955 1.00 39.09 113 O THR A 6426 -78.271 18.476 78.551 1.00 39.09 114 N TYR A 6527 -78.637 17.482 77.754 1.00 39.93 115 CA TYR A 6527 -80.016 16.771 76.044 1.00 39.93 116 CB TYR A 6527 -80.169 16.771 76.044 1.00 39.93 116 CB TYR A 6527 -79.698 17.921 75.211 1.00 39.35 119 CE1 TYR A 6527 -80.438 19.087 75.151 1.00 38.78 120	107	N	THR A	6426	-76.066	17.493	78.926	1.00	38.29
110 OG1 THR A 6426 -74.854 19.444 77.377 1.00 39.58 111 CG2 THR A 6426 -76.817 20.607 76.955 1.00 39.02 112 C THR A 6426 -79.066 19.157 79.198 1.00 39.04 114 N TYR A 6527 -78.637 17.482 77.754 1.00 39.93 115 CA TYR A 6527 -80.017 17.110 77.518 1.00 39.93 116 CB TYR A 6527 -80.169 16.771 76.044 1.00 39.52 117 CG TYR A 6527 -79.698 17.921 75.211 1.00 38.75 118 CD1 TYR A 6527 -80.006 20.166 74.431 1.00 39.27 120 C2 TYR A 6527 -78.800 21.180 73.049 1.00 38.76 121	108	CA	THR A	64 26	-76.761	18.725	78.622	1.00	38.88
111 CG2 THR A 6426 -76.817 20.607 76.955 1.00 39.02 112 C THR A 6426 -78.271 18.476 78.551 1.00 39.19 113 O THR A 6426 -79.066 19.157 79.198 1.00 39.04 114 N TYR A 6527 -78.637 17.482 77.754 1.00 39.93 115 CA TYR A 6527 -80.017 17.110 77.518 1.00 39.93 116 CB TYR A 6527 -80.169 16.771 76.044 1.00 39.35 117 CG TYR A 6527 -80.438 19.087 75.151 1.00 38.77 118 CD1 TYR A 6527 -80.006 20.166 74.431 1.00 39.35 119 CE1 TYR A 6527 -78.817 20.093 73.765 1.00 38.78 121	109	CB	THR A	64 26	-76.259	19.227	77.281	1.00	39.01
112 C THR A 6426 -78.271 18.476 78.551 1.00 39.19 113 O THR A 6426 -79.066 19.157 79.198 1.00 39.04 114 N TYR A 6527 -78.637 17.482 77.754 1.00 39.58 115 CA TYR A 6527 -80.017 17.110 77.518 1.00 39.52 116 CB TYR A 6527 -80.169 16.771 76.044 1.00 39.55 117 CG TYR A 6527 -79.698 17.921 75.151 1.00 38.77 118 CD1 TYR A 6527 -80.006 20.166 74.431 1.00 39.27 120 CZ TYR A 6527 -78.817 20.093 73.765 1.00 38.78 121 OH TYR A 6527 -78.051 18.947 73.817 1.00 38.83 123 <	110	OG1	THR A	6426	-74.854	19.444	77.377	1.00	39.58
113 O THR A 6426	111	CG2	THR A	6426	-76.817	20.607	76.955	1.00	39.02
114 N TYR A 6527 -78.637 17.482 77.754 1.00 39.58 115 CA TYR A 6527 -80.017 17.110 77.518 1.00 39.93 116 CB TYR A 6527 -80.169 16.771 76.044 1.00 39.52 117 CG TYR A 6527 -79.698 17.921 75.211 1.00 38.77 118 CD1 TYR A 6527 -80.006 20.166 74.431 1.00 39.37 120 CZ TYR A 6527 -78.817 20.093 73.765 1.00 38.78 121 OH TYR A 6527 -78.400 21.180 73.049 1.00 38.83 123 CD2 TYR A 6527 -78.488 17.878 74.549 1.00 38.83 123 CD2 TYR A 6527 -78.480 21.180 73.369 1.00 38.20 124	112	C	THR A	6426	-78.271	18.476	78.551	1.00	39.19
115 CA TYR A 6527	113	0	THR A	64 26	-79.066	19.157	79.198	1.00	39.04
116 CB TYR A 6527 -80.169 16.771 76.044 1.00 39.52 117 CG TYR A 6527 -79.698 17.921 75.211 1.00 38.77 118 CD1 TYR A 6527 -80.438 19.087 75.151 1.00 39.35 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 39.27 120 CZ TYR A 6527 -78.817 20.093 73.765 1.00 38.78 121 OH TYR A 6527 -78.400 21.180 73.049 1.00 38.94 122 CE2 TYR A 6527 -78.488 17.878 74.549 1.00 38.83 123 CD2 TYR A 6527 -80.398 15.926 78.368 1.00 40.73 124 C TYR A 6527 -80.398 15.926 78.368 1.00 40.73 125	114	N	TYR A	65 27	-78.637	17.482	77.754	1.00	39.58
117 CG TYR A 6527 -79.698 17.921 75.211 1.00 38.77 118 CD1 TYR A 6527 -80.438 19.087 75.151 1.00 39.35 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 39.27 120 CZ TYR A 6527 -78.817 20.093 73.765 1.00 38.78 121 OH TYR A 6527 -78.400 21.180 73.049 1.00 38.94 122 CE2 TYR A 6527 -78.480 17.878 74.549 1.00 38.20 124 C TYR A 6527 -80.398 15.926 78.368 1.00 40.73 125 O TYR A 6527 -80.207 14.793 77.969 1.00 41.03 126 N ARG A 6628 -81.271 15.065 80.420 1.00 43.55 128	115	CA	TYR A	65 27	-80.017	17.110	77.518	1.00	39.93
118 CD1 TYR A 6527 -80.438 19.087 75.151 1.00 39.35 119 CE1 TYR A 6527 -80.006 20.166 74.431 1.00 39.27 120 CZ TYR A 6527 -78.817 20.093 73.765 1.00 38.78 121 OH TYR A 6527 -78.400 21.180 73.049 1.00 38.94 122 CE2 TYR A 6527 -78.051 18.947 73.817 1.00 38.83 123 CD2 TYR A 6527 -78.488 17.878 74.549 1.00 38.20 124 C TYR A 6527 -80.398 15.926 78.368 1.00 40.73 125 O TYR A 6628 -80.207 14.793 77.969 1.00 41.03 126 N ARG A 6628 -81.271 15.065 80.420 1.00 43.55 128	116	CB	TYR A	65 27	-80.169	16.771	76.044	1.00	39.52
119 CE1 TYR A 6527	117	CG	TYR A	65 27	-79.698		75.211	1.00	38.77
120 CZ TYR A 6527 -78.817 20.093 73.765 1.00 38.78 121 OH TYR A 6527 -78.400 21.180 73.049 1.00 38.94 122 CE2 TYR A 6527 -78.481 18.947 73.817 1.00 38.83 123 CD2 TYR A 6527 -78.488 17.878 74.549 1.00 38.20 124 C TYR A 6527 -80.398 15.926 78.368 1.00 40.73 125 O TYR A 6527 -80.207 14.793 77.969 1.00 41.03 126 N ARG A 6628 -80.940 16.177 79.546 1.00 42.07 127 CA ARG A 6628 -81.271 15.065 80.420 1.00 43.55 128 CB ARG A 6628 -81.351 14.54 82.878 1.00 47.22 130 <	118	CD1	TYR A	65 27	~80.438	19.087	75.151	1.00	39.35
121 OH TYR A 6527 -78.400 21.180 73.049 1.00 38.94 122 CE2 TYR A 6527 -78.051 18.947 73.817 1.00 38.83 123 CD2 TYR A 6527 -78.488 17.878 74.549 1.00 38.20 124 C TYR A 6527 -80.398 15.926 78.368 1.00 40.73 125 O TYR A 6527 -80.207 14.793 77.969 1.00 41.03 126 N ARG A 6628 -80.940 16.177 79.546 1.00 42.07 127 CA ARG A 6628 -81.271 15.065 80.420 1.00 43.55 128 CB ARG A 6628 -81.423 15.521 81.873 1.00 44.02 129 CG ARG A 6628 -81.354 14.734 84.340 1.00 45.25 130	119		TYR A		-80.006	20.166			
122 CE2 TYR A 6527 -78.051 18.947 73.817 1.00 38.83 123 CD2 TYR A 6527 -78.488 17.878 74.549 1.00 38.20 124 C TYR A 6527 -80.398 15.926 78.368 1.00 40.73 125 O TYR A 6527 -80.207 14.793 77.969 1.00 41.03 126 N ARG A 6628 -80.940 16.177 79.546 1.00 42.07 127 CA ARG A 6628 -81.271 15.065 80.420 1.00 43.55 128 CB ARG A 6628 -81.423 15.521 81.873 1.00 44.02 129 CG ARG A 6628 -80.996 14.454 82.878 1.00 47.22 130 CD ARG A 6628 -81.354 14.734 84.340 1.00 55.65 132									
123 CD2 TYR A 6527		OH							
124 C TYR A 6527 -80.398 15.926 78.368 1.00 40.73 125 O TYR A 6527 -80.207 14.793 77.969 1.00 41.03 126 N ARG A 6628 -80.940 16.177 79.546 1.00 42.07 127 CA ARG A 6628 -81.271 15.065 80.420 1.00 43.55 128 CB ARG A 6628 -81.423 15.521 81.873 1.00 44.02 129 CG ARG A 6628 -81.423 15.521 81.873 1.00 47.22 130 CD ARG A 6628 -81.354 14.734 84.340 1.00 47.22 130 CD ARG A 6628 -81.354 14.734 84.699 1.00 51.56 131 NE ARG A 6628 -83.559 14.845 85.448 1.00 57.92 133 NH1 ARG A 6628 -83.291 16.050 85.930 1.00 58.60 </td <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>									
125 O TYR A 6527 -80.207 14.793 77.969 1.00 41.03 126 N ARG A 6628 -80.940 16.177 79.546 1.00 42.07 127 CA ARG A 6628 -81.271 15.065 80.420 1.00 43.55 128 CB ARG A 6628 -81.423 15.521 81.873 1.00 44.02 129 CG ARG A 6628 -81.423 15.521 81.873 1.00 44.02 130 CD ARG A 6628 -81.354 14.734 84.340 1.00 51.56 131 NE ARG A 6628 -82.668 14.202 84.699 1.00 55.65 132 CZ ARG A 6628 -83.559 14.845 85.448 1.00 57.92 133 NH1 ARG A 6628 -83.559 14.845 85.448 1.00 57.92 133 NH1 ARG A 6628 -83.291 16.050 85.930 1.00 58.60 134 NH2 ARG A 6628 -84.725 14.279 85.715 1.00 60.08 135 C ARG A 6628 -82.534 14.355 79.951 1.00 43.77 136 O ARG A 6628 -82.534 14.355 79.951 1.00 43.77 136 O ARG A 6628 -83.352 14.918 79.221 1.00 44.23 137 N LEU A 6729 -82.669 13.097 80.338 1.00 43.66 138 CA LEU A 6729 -82.669 13.097 80.338 1.00 43.66 138 CA LEU A 6729 -83.883 12.376 80.054 1.00 43.77 139 CB LEU A 6729 -83.883 12.376 80.054 1.00 43.77 139 CB LEU A 6729 -83.883 12.376 80.054 1.00 43.77 139 CB LEU A 6729 -83.893 10.758 78.121 1.00 44.26 141 CD1 LEU A 6729 -83.293 10.758 78.121 1.00 44.26 141 CD1 LEU A 6729 -82.836 9.324 77.850 1.00 45.40 142 CD2 LEU A 6729 -84.505 11.088 77.282 1.00 45.47				-					
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129 CG ARG A 6628 -80.996 14.454 82.878 1.00 47.22 130 CD ARG A 6628 -81.354 14.734 84.340 1.00 51.56 131 NE ARG A 6628 -82.668 14.202 84.699 1.00 55.65 132 CZ ARG A 6628 -83.559 14.845 85.448 1.00 57.92 133 NH1 ARG A 6628 -83.291 16.050 85.930 1.00 58.60 134 NH2 ARG A 6628 -84.725 14.279 85.715 1.00 60.08 135 C ARG A 6628 -82.534 14.355 79.951 1.00 43.77 136 O ARG A 6628 -83.352 14.918 79.221 1.00 44.23 137 N LEU A 6729 -82.669 13.097 80.338 1.00 43.66 138 CA LEU A 6729 -83.883 12.376 80.054 1.00 43.85<									
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136 O ARG A 6628 -83.352 14.918 79.221 1.00 44.23 137 N LEU A 6729 -82.669 13.097 80.338 1.00 43.66 138 CA LEU A 6729 -83.883 12.376 80.054 1.00 43.77 139 CB LEU A 6729 -83.602 10.950 79.602 1.00 43.85 140 CG LEU A 6729 -83.293 10.758 78.121 1.00 44.26 141 CD1 LEU A 6729 -82.836 9.324 77.850 1.00 45.40 142 CD2 LEU A 6729 -84.505 11.088 77.282 1.00 45.47									
137 N LEU A 6729 -82.669 13.097 80.338 1.00 43.66 138 CA LEU A 6729 -83.883 12.376 80.054 1.00 43.77 139 CB LEU A 6729 -83.602 10.950 79.602 1.00 43.85 140 CG LEU A 6729 -83.293 10.758 78.121 1.00 44.26 141 CD1 LEU A 6729 -82.836 9.324 77.850 1.00 45.40 142 CD2 LEU A 6729 -84.505 11.088 77.282 1.00 45.47									
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139 CB LEU A 6729 -83.602 10.950 79.602 1.00 43.85 140 CG LEU A 6729 -83.293 10.758 78.121 1.00 44.26 141 CD1 LEU A 6729 -82.836 9.324 77.850 1.00 45.40 142 CD2 LEU A 6729 -84.505 11.088 77.282 1.00 45.47									
140 CG LEU A 6729 -83.293 10.758 78.121 1.00 44.26 141 CD1 LEU A 6729 -82.836 9.324 77.850 1.00 45.40 142 CD2 LEU A 6729 -84.505 -11.088 77.282 1.00 45.47									
141 CD1 LEU A 6729 -82.836 9.324 77.850 1.00 45.40 142 CD2 LEU A 6729 -84.505 11.088 77.282 1.00 45.47									
142 CD2 LEU A 67 29 -84.505 11.088 77.282 1.00 45.47									
	143								

FIGURE 3-(Cont.)C

A	В	C I) E	F	G	Н	I	J
144	0	LEU A	4 67 29	-83.983	12.028	82.397	1.00	43.27
145	N	LYS A	68 30	-85.831	12.804	81.393		43.83
146	CA	LYS A		-86.540	12.864	82.653		44.19
147	CB	LYS A		-87.558	13.999	82.623	1.00	44.45
148	CG	LYS A	68 30	-87.589	14.791	83.904		45.86
149	CD	LYS A	6830	-87.585	16.278	83.631		48.33
150	CE	LYS A	6830	-87.850	17.057	84.915	1.00	50.36
151	NZ	LYS A	68 30	-87.184	16.414	86.093	1.00	50.63
152	C	LYS A	6830	-87.188	11.530	82.992	1.00	43.80
153	0	LYS A	. 68 30	-87.671	10.828	82.119	1.00	43.69
154	N	LEU A	69 31	-87.176	11.182	84.269	1.00	43.81
155	CA	LEU A	69 31	-87.756	9.930	84.734	1.00	43.79
156	CB	LEU A	. 69 31	-86.736	9.163	85.574	1.00	43.75
157	CG	LEU A	69 31	-85.603	8.328	84.969	1.00	44.56
158	CD1	LEU A	. 69 31	-84.873	9.055	83.846	1.00	43.44
159	CD2	LEU A	69 31	-84.628	7.930	86.096	1.00	44.48
160	C	LEU A	69 31	-88.977	10.156	85.617	1.00	43.68
161	0	LEU A	69 31	-89.333	11.277	85.963	1.00	43.78
162	N	TYR A	70 32	-89.615	9.065	85.996	1.00	43.53
163	CA	TYR A	7032	~90.674	9.138	86.968	1.00	43.23
164	CB	TYR A		-92.052	9.303	86.338	1.00	43.05
165	CG	TYR A	70 32	-93.048	9.809	87.349	1.00	42.24
166	CD1	TYR A	70 32	-93.511	8.981	88.365	1.00	40.80
167	CE1	TYR A	70 32	~94.404	9.431	89.295	1.00	40.31
168	CZ	TYR A	70 32	-94.844	10.741	89.243	1.00	41.67
169	OH	TYR A		~95.739	11.185	90.191	1.00	43.57
170	CE2	TYR A	70 32	-94.393	11.593	88.260	1.00	41.02
171	CD2	TYR A	70 32	-93.490	11.127	87.321	1.00	41.49
172	C	TYR A	70 32	-90.607	7.874	87.767		43.22
173	0	TYR A	70 32	-91.398	6.966	87.573	1.00	43.16
174	N	SER A	7133	-89.646	7.823	88.671	1.00	43.72
175	CA	SER A	71 33	-89.442	6.642	89.486	1.00	44.29
176	CB	SER A	71 33	-87.971	6,494	89.860	1.00	44.28
177	OG	SER A	7133	-87.829	5.415	90.769	1.00	45.94
178	C	SER A	71 33	-90.255	6.707	90.749	1.00	44.40
179	0	SER A	$\frac{71}{33}$	-90.016	7.558	91.591	1.00	44.77
180	N	LEU A	72 <u>34</u>	-91.195	5.782	90.895		44.57
181	CA	LEU A	72 34	-92.057	5.761	92.058	1.00	44.62
182	CB	LEU A	72 34	-93.520	5.959	91.626	1.00	
183	CG	LEU A	72 34	-94.125	4.942	90.643		43.66
184	CD1	LEU A	7234	-94.404	3.595	91.314		40.76
185	CD2	LEU A	7234	-95.392	5.481	89.957		41.85
186	C	LEU A	72 34	-91.893	4.444	92.788		45.36
187	0	LEU A	7234	-91.354	3.490	92.236		45.44
188	N	ARG A	73 35	-92.332	4.398	94.038		46.33
189	CA	ARG A	73 35	-92.342	3.152	94.780		48.23
190	CB	ARG A	73 35	-91.397	3.171	95.983	1.00	
191	CG	ARG A	73 35	-90.088	3.873	95.758	1.00	
192	CD	ARG A	73 35	-89.158	3.812	96.952	1.00	
193	NE	ARG A	73 <u>35</u>	-87.815	4.235	96.585	1.00	
194	CZ	ARG A	73 35	-86.755	4.134	97.378	1.00	53.95

FIGURE 3-(Cont.)D

A	В	C I	E	P	G	Н	Ĭ	J
195	NHl	ARG A	7335	-86.886	3.625	98.600	1.00	51.85
196	NH2	ARG A		-85.569	4.552	96.942		53.73
197	C	ARG A		-93.743	3.011	95.297	1.00	
198	O	ARG A		-94.246	3.909	95.958	1.00	
199	N	TRP A		-94.381	1.891	95.009	1.00	
200	CA	TRP A		-95.722	1.688	95.504		50.47
201	CB	TRP A		-96.409	0.550	94.751		50.15
202	CG	TRP A		-96.845	0.918	93.357	1.00	
203	CD1	TRP A	7436	-96.282	0.500	92.191	1.00	
204	NE1	TRP A	7436	-96.956	1.033	91.120	1.00	48.90
205	CE2	TRP A	7436	-97.985	1.813	91.581	1.00	48.49
206	CD2	TRP A		-97.945	1.765	92.987	1.00	48.80
207	CE3	TRP A	7436	-98.902	2.490	93.704	1.00	48.56
208	CZ3	TRP A	7436	-99.857	3.220	93.005	1.00	49.05
209	CH2	TRP A	7436	-99.867	3.246	91.607	1.00	47.62
210	CZ2	TRP A	7436	-98.940	2.553	90.879	1.00	48.27
211	C	TRP A	7436	-95.581	1.359	96.970	1.00	51.34
212	0	TRP A	7436	-94.558	0.821	97.388	1.00	51.46
213	N	ILE A	75 37	-96.598	1.685	97.757	1.00	52.47
214	CA	ILE A	7537	-96.559	1.421	99.191	1.00	53.41
215	CB	ILE A	75 37	-96.449	2.737	99.958	1.00	53,42
216	CG1	ILE A	75 37	-94.987	3.025	100.270	1.00	53.87
217	CD1	ILE A	7537	-94.196	3.466	99.076	1.00	54.40
218	CG2	ILE A	7537	-97.246	2.685	101.244	1.00	54.45
219	C	ILE A	75 37	-97.793	0.648	99.612	1.00	53.93
220	0	ILE A	75 37	-97.812	-0.066	100.617	1.00	53.82
221	N	SER A	76 38	-98.833	0.793	98.814	1.00	54.88
222	CA	SER A	76 38	-100.072	0.103	99.078	1.00	55.80
223	CB	SER A	76 38	-101.023	1.013	99.840	1.00	55.67
224	OG	SER A	76 38	-100.863	2.357	99.413	1.00	56.45
225	С	ser a	76 38	-100.650	-0.235	97.731	1.00	56.36
226	0	SER A	76 38	-99.944	-0.241	96.726	1.00	56.35
227	N	ASP A	77 39	-101.945	-0.488	97.696	1.00	57.13
228	CA	ASP A	77 39	-102.560	-0.803	96.435	1.00	57.78
229	CB	ASP A	77 39	-103.718	-1.766	96.627		58.12
230	CG	ASP A	77 39	-103.988	-2.578	95.392		59.53
231	OD1	ASP A	7739	-105.111	-3.106	95.254	1.00	61.71
232	OD2	ASP A	77 39	-103.127	-2.745	94.500		61.65
233	C	ASP A	77 39	-103.046	0.452	95.753		57.97
234	0	ASP A	7739	-103.764	0.363	94.767		58.27
235	N	HIS A	78 40	-102.660	1.620	96.261	1.00	
236	CA	HIS A	7840	-103.128	2.865	95.654	1.00	
237	CB	HIS A	78 40	-104.625	3.072	95.920	1.00	
238	CG	HIS A	7840	-105.071	2.575	97.257	1.00	
239	ND1	HIS A	78 <u>40</u>	-106.098	1.666	97.409	1.00	
240	CEl	HIS A	7840	-106.264	1.405	98.694	1.00	
241	NE2	HIS A	78 40	-105.379	2.107	99.380	1.00	
242	CD2	HIS A	78 40	-104.618	2.845	98.504	1.00	
243 244	C 0	HIS A	78 40 78 40	-102.354 -102.744	4.110	96.059 95.720	1.00	
	N	GLU A			5.229		1.00	
245	7.4	M ULL	79 41	-101.259	3.915	96.780	1.00	50.00

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FIGURE 3-(Cont.)E

A	В	C :	D E	F	G	H	Ι	J
246	CA	GLU	A 7941	-100.409	5.027	97,167	1.00	57.73
247	CB	GLU 2	A 7941	-100.372	5.162	98.690		57.77
248	CG	GLU Z	P-4-4-4-	-101.698	5.542	99.334		57.46
249	CD	GLU 1		~101.505	6.168	100.703		56.70
250	OE1	GLU 1		-101.106	5.438	101.644		56.35
251	OE2	GLU Z	*****	-101.736	7.391	100.832		55.22
252	C	GLU A	A 7941	-99.002	4.787	96.645		57.49
253	0	GLU A	A 7941	-98.593	3.642	96.493		57.77
254	N	TYR A	8042	-98.256	5.849	96.370		57.25
255	CA	TYR A	4 8042	-96.869	5.669	95.954	1.00	57.17
256	CB	TYR A	4 80 42	-96.776	5.319	94.471	1.00	56.71
257	CG	TYR A	8042	-97.027	6.456	93.510	1.00	54.55
258	CD1	TYR A	8042	~96.053	7.407	93.272	1.00	52.96
259	CEl	TYR A	8042	-96.254	8.430	92.382	1.00	51.65
260	CZ	TYR A	8042	-97.440	8.513	91.693	1.00	51.43
261	OH	TYR A	8042	-97.622	9.545	90.803	1.00	49.55
262	CE2	TYR A	80 <u>42</u>	-98.427	7.572	91.897	1.00	52.02
263	CD2	TYR A	8042	-98.215	6.546	92.802	1.00	53.03
264	C	TYR A	8042	-95.948	6.837	96.294	1.00	57.82
265	0	TYR A	8042	-96.333	8.003	96.191	1.00	57.89
266	N	LEU A	81 <u>43</u>	-94.723	6.510	96.688	1.00	58.48
267	CA	LEU A	8143	-93.746	7.526	97.049	1.00	59.28
268	CB	LEU A	81 43	-92.773	6.996	98.103	1.00	59.23
269	CG	LEU A	8143	-93.436	6.643	99.433	1.00	58.97
270	CD1	LEU A		-92.447	6.044	100.404	1.00	57.55
271	CD2	LEU A	8143	-94.111	7.874	100.016	1.00	58.52
272	С	LEU A	81 <u>43</u>	-92.975	8.011	95.849	1.00	59.92
273	O	LEU A	**********	-92.592	7.230	94.989	1.00	60.06
274	N	TYR A	white makes of	-92.762	9.318	95.799	1.00	61.07
275	CA	TYR A		-91.976	9.941	94.749	1.00	62.31
276	CB	TYR A		-92.881	10.720	93.798	1.00	61.95
277	CG	TYR A	vaccour	-92.187	11.345	92.608	1.00	61.54
278	CD1	TYR A		-91.690	10.561	91.569	1.00	61.21
279	CE1	TYR A		-91.058	11.136	90.474	1.00	60.70
280	CZ	TYR A	***************************************	-90.923	12.508	90.414	1.00	61.23
281	OH	TYR A		-90.301	13.098	89.336	1.00	61.42
282	CE2	TYR A		~91.411	13.303	91.433	1.00	60.86
283	CD2	TYR A		-92.038	12.722	92.516	1.00	61.00
284	C	TYR A	82 44	-91.030	10.867	95.492	1.00	63.51
285	0	TYR A	8244	-91.299	11.226	96.634	1.00	63.78
286	N	LYS A	***************************************	-89.916	11.232	94.873		65.00
287	CA	LYS A		-88.948	12.098	95.532		66.61
288	CB	LYS A	8345	-87.641	11.335	95.779		66.63
289	CG	LYS A	83 45	-86.657	12.048	96.701		67.24
290	CD	LYS A	8345	-85.319	11.316	96.767		68.31
291	CE	LYS A	8345	-84.269	12.139	97.509		68.73
292	NZ	LYS A	83<u>45</u>	-84.810	12.690	98.791		69.48
293	C	LYS A	83<u>45</u>	-88.702	13.332	94.671	1.00	
294	0	LYS A	83 45	~88.234	13.207	93.540	1.00	
295	N	GLN A	84 46	-89.017	14.518	95.198	1.00	
296	CA	GLN A	84 46	-88.868	15.752	94.415	1.00	70.27

FIGURE 3-(Cont.)F

A	В	C D	E	F	G	H	I	Ĵ
297	СВ	GLN A	8446	-90.210	16.495	94.254	1.00	70.38
298	CG	GLN A		-90.189	17.523		1.00	
299	CD	GLN A	***************************************	-91.574	18.038		1.00	
300	OE1	GLN A	-	-92.566	17.300		1.00	
301	NE2	GLN A		-91.637	19.308		1.00	
302	C	GLN A	8445	-87,771	16.710		1.00	
303	0	GLN A	8446	-88.012	17.595		1.00	
304	N	GLU A	8547	-86.569	16.518		1.00	
305	CA	GLU A	85 47	~85.413	17.393	94.580	1.00	72,37
306	CB	GLU A	85 47	-85.480	18.608	93.644	1.00	72.68
307	CG	GLU A	85 47	-85.040	18.336	92.211	1.00	73.91
308	CD	GLU A	8547	-83.561	18.604	91.986	1.00	75.82
309	OEl	GLU A	8547	-83.116	19.761	92.179	1.00	76.43
310	OE2	GLU A	85 47	-82.840	17.657	91.612	1.00	76.92
311	C	GLU A	85 47	-85.240	17.869	96.019	1.00	72.44
312	0	GLU A	85 47	-84.595	18.894	96.268	1.00	72.64
313	N	ASN A	86 48	~85.801	17.116	96.959	1.00	72.46
314	CA	ASN A	86 48	-85.737	17.471	98.368	1.00	72.28
315	CB	ASN A	86 48	-86.404	18.833	98.599	1.00	72.52
316	CG	asn a	$\frac{8648}{1}$	-85.409	19.943	98.933	1.00	73.27
317	OD1	ASN A	8648	-84.235	19.690	99.213	1.00	74.24
318	ND2	ASN A	86 48	-85.890	21.185	98.919	1.00	73.24
319	С	asn a	86 48	-86.443	16.444	99.243	1.00	72.00
320	0	ASN A	86 48	-85.861		100.186	1.00	72.38
321	N-	ASN A	8749	-87.695	16.158	98.902	1.00	71.24
322	CA	ASN A	87 49	-88.567	15.415	99.796	1.00	70.45
323	CB	ASN A	8749	-89.521	16.417	100.442	1.00	70.52
324	CG	ASN A	8749	-90.018	17.461	99.449	1.00	70.98
325	OD1	ASN A	87 <u>49</u>	-90.640	18.460	99.828	1.00	70.94
326	ND2	ASN A	87 <u>49</u>	-89.742	17.233	98.166	1.00	70.86
327 328	C O	ASN A ASN A	87 49 87 49	-89.396 -89.781	14.293	99.200	1.00	69.91
329	N	ILE A	88 50		14.321	98.028	1.00	70.04
330	CA	ILE A	88 50	-89.701 -90.539	13.316		1.00	69.04
331	CB	ILE A	88 50	-90.337	11.008	99.641 100.573	1.00	68.26 68.17
332	CG1	ILE A	8 850	-88.957	10.390	100.357		68.29
333	CD1	ILE A	88 50	-87.916	10.833	101.355		68.40
334	CG2	ILE A	88 50	-91.408		100.328		68.21
335	C	ILE A	88 50	-92.001	12.622	99.655	1.00	67.54
336	ō	ILE A	88 50	-92.544		100.696	1.00	67.50
337	N	LEU A	89 51	-92.628	12.586	98.488		66.76
338	CA	LEU A	89 51	-94.043	12.899	98.366		65.98
339	CB	LEU A	89 51	-94.323	13.580	97.024	1.00	
340	CG	LEU A	89 51	-94.640	15.082	97.012	1.00	
341	CDI	LEU A	89 51	-93.931	15.820	98.139	1.00	
342	CD2	LEU A	89 51	-94.322	15.711	95.652	1.00	
343	C	LEU A	89 51	-94.859	11.621	98.471	1.00	
344	0	LEU A	89 51	-94.350	10.533	98.225	1.00	65.35
345	N	VAL A	9052	-96.119	11.748	98.869	1.00	
346	CA	VAL A	90 52	-97.026	10.608	98.869	1.00	
347	CB	VAL A	90 52	-97.772	10.450	100.184	1.00	64.07

FIGURE 3-(Cont.)G

Α	В	C D	E	F	G	Н	I	J
348	CG1	VAL A	90 52	-97.047	11.166	101.304	1.00	64.22
349	CG2	VAL A	9052	-98.002	8.966	100.488	1.00	63.60
350	C	VAL A	90 52	-98.082	10.913	97.839	1.00	63.33
351	0	VAL A	90 52	-98.626	12.013	97.823	1.00	63.43
352	N	PHE A	91 53	-98.383	9.949	96.981	1.00	62.56
353	CA	PHE A	91 53	-99.390	10.165	95.959	1.00	61.64
354	CB	PHE A	91 53	-98.778	10.047	94.569	1.00	61.67
355	CG	PHE A	91 53	-98.025	11.265	94.117	1.00	61.05
356	CD1	PHE A	91 53	-96.751	11.523	94.586	1.00	61.29
357	CEL	PHE A	91 53	-96.053	12.634	94.151	1.00	61.02
358	CZ	PHE A	91 53	-96.625	13.495	93.236	1.00	60.95
359	CE2	PHE A	91 53	-97.892	13.244	92.756	1.00	60.57
360	CD2	PHE A	91 53	-98.580	12.130	93.192	1.00	60.71
361	C	PHE A	91 53	-100.505	9.150	96.078	1.00	61.31
362	0	PHE A	91 53	-100.254	7.965	96.304	1.00	61.35
363	N	ASN A	92 54	-101.742	9.620	95.960	1.00	60.84
364	ÇA	ASN A	92 54	-102.876	8.717	95.857	1.00	60.32
365	CB	ASN A	92 54	-104.179	9.395	96.288	1.00	60.41
366	CG	asn a	92 54	-105.340	8.409	96.429	1.00	60.97
367	OD1	ASN A	92 54	-106.103	8.477	97.390		61,46
368	ND2	asn a	92 54	-105.477	7.493	95.470	1.00	60,70
369	C	asn a	92 54	-102.936	8.393	94.382	1.00	59.76
370	0	ASN A	92 54	-102.896	9.295	93.543	1.00	59.60
371	Ŋ	ALA A	93 55	-103.004	7.115	94.047	1.00	59.38
372	CA	ALA A	93 55	-103.065	6.740	92.641	1.00	59.02
373	CB	ALA A	93 55	-102.952	5.237	92.488	1.00	59.06
374	C	ALA A	93 55	-104.322	7.276	91.937	1.00	58.71
375	0	ALA A	93 55	-104.242	7.767	90.816		58.09
376	N	GLU A	94 56	-105.473	7.195	92.598	1.00	58.94
377	CA	GLU A	94 56	-106.736	7.646	91.991	1.00	59.29
378	CB	GLU A	94 56	-107.930	7.354	92.906	1.00	59.17
379	CG	GLU A	94 56	-108.493	5.948	92.791	1.00	59.64
380	CD	GLU A	9456	-109.508	5.794	91.670	1.00	59.62
381	OE1	GLU A	94 56	-109.458	6.558	90.681	1.00	59.64
382	OE2	GLU A	94 56	-110.371	4.904	91.782	1.00	59.77
383	C	GLU A	94 56	-106.787	9.115	91.563		59.42
384	0	GLU A	9456	-107.172	9.421	90.434		59.29
385	N	TYR A	95 57	-106.388	10.023	92.448		59.76
386	CA	TYR A	95 <u>57</u>	-106.556	11.453	92.162		60.14
387	CB	TYR A	9557	-107.191	12.151	93.365		60.19
388	CG	TYR A	9557 0557	-108.191 -109.455	11.284	94.093	1.00	
389	CD1	TYR A	9557		11.059	93.565	1.00	
390	CE1	TYR A	95 <u>57</u>	-110.373	10.267	94.226	1.00	
391	CZ	TYR A	95 <u>57</u>	-110.030	9.676	95.425	1.00	
392	OH CE2	TYR A	95 57 9557	-110.941	8.877	96.072	1.00	
393	CE2	TYR A	W-9900-000	-108.775 -107.865	9.871	95.966	1.00	
394 395	CD2	TYR A TYR A	95 57 95 57	-107.865 -105.297	10.677	95.299 91.743		
395	0	TYR A	MATERIAL DE LA CONTRACTOR DE LA CONTRACT		12.200		1.00	
397	N	GLY A	95 57 9658	-105.382 -104.132	13.286 11.630	91.170 92.037	1.00	
398	CA	GLY A	9658	-104.132	12.281	91.700	1.00	
J J U	4.3	-44 tJ	~~ <u>~~</u>	102.001		72.740	7.70	· · · * 4